Periodic features in the Dynamic Structure Factor of the Quasiperiodic Period-doubling Lattice

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We present an exact real-space renormalization group (RSRG) method for evaluating the dynamic structure factor of an infinite one-dimensional quasiperiodic period-doubling (PD) lattice. We observe that for every normal mode frequency of the chain, the dynamic structure factor $S(q,\omega)$ always exhibits periodicity with respect to the wave vector q and the presence of such periodicity even in absence of translational invariance in the system is quite surprising. Our analysis shows that this periodicity in $S(q,\omega)$ actually indicates the presence of delocalized phonon modes in the PD chain. The Brillouin Zones of the lattice are found to have a hierarchical structure and the dispersion relation gives both the acoustic as well as optical branches. The phonon dispersion curves have a nested structure and we have shown that it is actually the superposition of the dispersion curves of an infinite set of periodic lattices.

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I. INTRODUCTION

The discovery of icosahedral phase in Al-Mn alloys by Shechtman et al. [1] initiated experimental and theoretical research on quasiperiodic systems. Theoretical investigations are mostly based on one-dimensional quasiperiodic systems, as they can be described by simple models for pointing out the relevant properties of these systems. There are many interesting works in the literature concerning the electronic [2–9] and vibrational properties [10–15] of these lattices. At present there is considerable amount of understanding about the nature of the eigenfunctions and the eigenvalue spectrum for this class of deterministic hierarchical systems lacking translational invariance. The general consensus is that the properties like critical states, Cantor-set spectrum, power-law behavior of the density of states etc. [3,8] are the characteristic features of the quasiperiodic or aperiodic systems, though there are evidences of extended states [5,7] in such systems. Moreover, there are also some reports on the anomalous transport [8] and optical localization [9] properties of these systems. But so far very less attention has been given regarding the dynamic response function of these lattices, a quantity which is directly connected to the scattering cross-section obtained from neutron diffraction or X-ray scattering experiments. Even the computation of the dynamic structure factor for one-dimensional quasiperiodic system is quite meaningful, as it is now possible to fabricate semiconducting superlattices epitaxially [16], and one can perform neutron diffraction or X-ray scattering experiments on these samples. Therefore, we can directly compare the theoretical predictions with the experimental results. As we will see, the study of the dynamic structure factor also gives information about the nature of the eigenmodes and consequently one can predict the character of the modes from experimental observations.

In this paper we have addressed the dynamical properties of quasiperiodic systems. We have computed the dynamical structure factor for the quasiperiodic period-doubling (PD) chain using a technique based on the real-space renormalization group (RSRG) method. Here we present a formalism for calculating the dynamic structure factor of the system using ideas developed in Ref. [12]. This is an exact method for computing the dynamic structure factor for a class of one-dimensional quasiperiodic chains, where the original lattice can be split into a finite number of self-similar sublattices.

Our study of the dynamic structure factor also gives information about the nature of the eigenmodes. The dispersion relation for the PD chain can be easily obtained from the dynamic structure factor, and the normal mode frequencies become readily available. Hence it is possible to characterize the nature of the states using the transfer matrix technique. The most interesting observation is that for every normal mode frequency of the PD chain, the dynamic structure factor becomes a periodic function of the wavevector, and it actually signifies that this lattice supports delocalized classical vibrational modes for all these eigenmodes. We have also shown that for a certain choice of the parameters of the system, the dynamics of the PD chain exactly coincide with that of various periodic chains having different periods, and the corresponding features are reflected in the dispersion relation. Our study also reveals that one can infer about the delocalized nature of the states from a mere inspection of the X-ray or neutron scattering experiment data.

In this work, though we have concentrated our attention on the quasiperiodic PD chain, the ideas are quite general

and will be applicable in many other quasiperiodic systems. We have studied the PD chain as a prototype example for illustrating our method. An added interest in taking the PD lattice is that the problem of the existence of delocalized modes in this lattice can also be studied on the basis of dimmer-type correlation [5,17] among the atoms. But we would like to stress that though the method of Ref. [5] is theoretically very elegant, from the practical point of view its applicability is highly limited. The procedure of Ref. [5] actually gives only few delocalized normal mode frequencies, and the determination of the entire spectrum becomes a formidable computational task as it requires the solutions of polynomial equations with progressively higher and higher degree. On the other hand, the dynamic structure factor automatically gives the entire spectrum and the nature of the eigenmode corresponding to every normal mode frequency can be easily characterized. An interesting feature of the PD chain is that the trace map associated with this lattice leads to a polynomial invariant which should normally ensure the critical nature of all the eigenstates as well as a Cantor-set spectrum [3,10]. However, in this work we find that this lattice supports an infinity of delocalized states in spite of the Cantor-set nature of the spectrum.

This paper has been organized as follows. We first describe our model in Section II. We present in Section III the RSRG scheme for finding the dynamic structure factor of a quasiperiodic system, while we briefly outline the transfer matrix method in the next Section. Section V is devoted for the analysis of our results and we conclude in Section VI.

II. DESCRIPTION OF THE MODEL

We describe the vibrational properties of the PD chain considering nearest neighbor harmonic interaction among the atoms. A portion of the PD chain is shown in Fig. 1. The PD sequence can be generated from two symbols L and S using recursively the substitution rule $L \rightarrow LS$ and $S \rightarrow LL$. Thus L, LS, $LSLL$, $LSLLLSLS$, ... etc. are the first few generations of the PD sequence. Now we can construct a PD chain by considering the symbols L and S as representing 'long' (L) and 'short' (S) bonds in the chain. In our model m_α, m_β and m_γ are the masses of the atoms flanked by $L-L$, $L-S$ and $S-L$ bonds respectively, and, k_L and k_S are respectively the spring constants across the long and short bonds. It should be noted that this kind of labeling of the sites and the bonds is essential for implementing the RSRG decimation procedure of Southern et al. [18]. We shall see that successive renormalized lattices can be represented in terms of only these five parameters and the number of the parameters do not grow with iteration. In other words, within this labeling scheme, the form of the equations of motion of the system remains invariant under renormalization. The well-known on-site model and the bond-model for the PD chain turn out to be the special cases of this general situation.

The expression for the dynamic structure factor $S(q,\omega)$ corresponding to the wavevector q and frequency ω can be written in terms of the single particle Green's functions as follows

$$S(q,\omega) = \lim_{\delta \rightarrow 0^+} \lim_{N \rightarrow \infty} \mathrm{Im}(G_N(q,\omega+i\delta)) \ , \tag{1}$$

where $G_N(q,\omega) = (1/N)\sum_{ij} e^{iq(r_i-r_j)} G_{ij}$. Here r_i is the position vector of the ith atom and N represents the total number of atoms in the chain. In the harmonic approximation with nearest neighbor coupling between the atoms, the single particle Green's functions G_{ij}'s satisfy the following equations of motion

$$\epsilon_i G_{ij} = -\delta_{ij} + k_{i,i+1} G_{i+1j} + k_{i,i-1} G_{i-1j} \ , \tag{2}$$

where $\epsilon_i = k_{i,i+1} + k_{i,i-1} - m_i\omega^2$, m_i being the mass of the ith atom, and k_{ij} the spring constant between the ith and jth atoms.

Now the calculation of $S(q,\omega)$ for a translationally invariant system is very straight forward. $G_N(q,\omega)$ can be easily computed from a Fourier transformed version of the Eqs. (2). However, for quasiperiodic systems the determination of the sum in $G_N(q,\omega)$ is not trivial. We shall show in the next section that this sum can be evaluated in a very elegant way using RSRG method. The calculation of $S(q,\omega)$ essentially amounts to the iteration of certain recursion relations and it can be computed with arbitrarily high accuracy.

III. RSRG SCHEME FOR THE DETERMINATION OF $S(Q,\omega)$

Let us now consider the sum $G^i(q,\omega) = \sum_j e^{iq(r_i-r_j)} G_{ij}$. This sum is independent of the index i in a periodic system due to the translational invariance. However, in the case of a quasiperiodic system, it depends on the index i as no two sites are equivalent in the quasiperiodic lattice and from Eqs. (2) we obtain

$$\epsilon_i G^i(q,\omega) = -F_i + k_{i,i+1}e^{-iq(r_{i+1}-r_i)}G^{i+1}(q,\omega) + k_{i,i-1}e^{iq(r_i-r_{i-1})}G^{i-1}(q,\omega) \ , \tag{3}$$

where all F_i's are initially equal to unity. The use of new notations F_i's for representing unity does not directly follow from Eqs. (2). We have introduced these notations by hand and we will see how it facilitates the determination of $S(q,\omega)$ in quasiperiodic lattices. Even though all F_i's are initially the same, they become different upon renormalization. However, from the symmetry of the lattice, we observe that there will be only three distinct type of F_i's, and we can identify them as F_α, F_β and F_γ corresponding to the α, β and γ site of the lattice.

It is now necessary to determine all $G^i(q,\omega)$'s from Eqs. (3) for evaluating $G_N(q,\omega)$ since we have

$$G_N(q,\omega) = (1/N)\sum_i G^i(q,\omega) \ . \tag{4}$$

In the quasiperiodic PD chain $G^i(q,\omega)$'s are all distinct and instead of determining them directly from Eqs. (3), we use RSRG technique for finding them. We split the original chain into two self-similar sublattices Ω and Γ as shown in Fig. 1. The Ω-sublattice is obtained by eliminating the sites using the decimation rules $LS \rightarrow L$ and $LL \rightarrow S$, while the corresponding rules for the Γ-sublattice are $SL \rightarrow L$ and $LL \rightarrow S$. Both Ω and Γ sublattices again form two new PD chains at some inflated length scale. All the sites of the original PD lattice are distributed among these two sublattices, and thus they are complementary to each other (see Fig. 1). This complementary nature of Ω and Γ sublattices also ensures that no information is lost by introducing this splitting procedure. It is now possible to generate two sets of renormalized equations for $G^i(q,\omega)$'s, one corresponding to Ω-sublattice while the other for the Γ-sublattice. The equations for Ω-sublattice can be obtained from Eqs. (3) by eliminating all $G^i(q,\omega)$'s belonging to the Γ-sublattice, and the resulting equations can be cast in the same form as that of the original set of equations (3), provided we rename the sites appropriately and renormalize the parameters as follows

$$\begin{aligned}
\epsilon_\alpha^{'} &= \epsilon_\gamma - \omega_\beta(k_L^2 + k_S^2), \\
\epsilon_\beta^{'} &= \epsilon_\gamma - (k_L^2\omega_\alpha + k_S^2\omega_\beta), \\
\epsilon_\gamma^{'} &= \epsilon_\alpha - k_L^2(\omega_\alpha + \omega_\beta), \\
F_\alpha^{'} &= F_\gamma + F_\beta k_S\omega_\beta e^{iqa_S} + F_\beta k_L\omega_\beta e^{-iqa_L}, \\
F_\beta^{'} &= F_\gamma + F_\alpha k_L\omega_\alpha e^{-iqa_L} + F_\beta k_S\omega_\beta e^{iqa_S}, \\
F_\gamma^{'} &= F_\alpha + F_\alpha k_L\omega_\alpha e^{iqa_L} + F_\beta k_L\omega_\beta e^{-iqa_L}, \\
k_L^{'} &= k_L k_S\omega_\beta \ , \\
k_S^{'} &= k_L^2\omega_\alpha \ , \\
a_L^{'} &= a_L + a_S \ , \\
a_S^{'} &= a_L + a_L \ .
\end{aligned} \tag{5}$$

Similarly for the Γ-sublattice the recursion relations can be written as

$$\begin{aligned}
\epsilon_\alpha^{'} &= \epsilon_\beta - \omega_\gamma(k_L^2 + k_S^2), \\
\epsilon_\beta^{'} &= \epsilon_\alpha - k_L^2(\omega_\alpha + \omega_\gamma), \\
\epsilon_\gamma^{'} &= \epsilon_\beta - (k_S^2\omega_\gamma + k_L^2\omega_\alpha), \\
F_\alpha^{'} &= F_\beta + F_\gamma k_L\omega_\gamma e^{iqa_L} + F_\gamma k_S\omega_\gamma e^{-iqa_S}, \\
F_\beta^{'} &= F_\alpha + F_\beta k_L\omega_\alpha e^{-iqa_L} + F_\gamma k_S\omega_\gamma e^{iqa_S}, \\
F_\gamma^{'} &= F_\beta + F_\alpha k_L\omega_\alpha e^{iqa_L} + F_\gamma k_S\omega_\gamma e^{-iqa_S}, \\
k_L^{'} &= k_L k_S\omega_\gamma \ , \\
k_S^{'} &= k_L^2\omega_\alpha \ , \\
a_L^{'} &= a_L + a_S \ , \\
a_S^{'} &= a_L + a_L \ .
\end{aligned} \tag{6}$$

Here $\epsilon_i = k_{i,i+1} + k_{i,i-1} - m_i\omega^2$, $\omega_i = 1/\epsilon_i$ and i refers to α, β or γ. In Eqs. (5) and (6) a_L and a_S respectively represent the 'long' and 'short' bond lengths. Let us represent the above two transformations by $T_{\Omega(\Gamma)}$ and denote the renormalized Green's functions as $G^i_{\Omega(\Gamma)}$. Now we can recast $G_N(q,\omega)$ as

$$G_N(q,\omega) = p_{(\Omega)} G_N^{(\Omega)}(q,\omega) + p_{(\Gamma)} G_N^{(\Gamma)}(q,\omega), \tag{7}$$

where $G_N^{(\lambda)}(q,\omega) = (1/N_\lambda)\sum_{i\in\lambda} G^i_{(\lambda)}(q,\omega)$. Here λ can be either Ω or Γ, and $N_{\Omega(\Gamma)}$ is the number of sites in the renormalized $\Omega(\Gamma)$ sublattice. The coefficients $p_{(\Omega)}$ and $p_{(\Gamma)}$ denote the fractions of total sites which belong to Ω and Γ sublattices respectively, i.e., $p_{(\Omega)} = N_\Omega/N$ and $p_{(\Gamma)} = N_\Gamma/N$. The expressions for $G_N(q,\omega)$ and $G_N^{(\lambda)}(q,\omega)$ are structurally same, the former being defined in terms of the parameters of the original PD lattice while the latter refers to those of the renormalized λ-sublattice. Eq. (7) shows that $G_N(q,\omega)$ is a linear combination of $G_N^{(\Omega)}(q,\omega)$ and $G_N^{(\Gamma)}(q,\omega)$ with coefficients $p_{(\Omega)}$ and $p_{(\Gamma)}$, where $p_{(\Omega)} = p_{(\Gamma)} = 1/2$. Since each of these sublattices again forms a new PD chain, we can treat them at the same footing as the original chain. Thus in the renormalized $\Omega(\Gamma)$ sublattice, $G_N^{\Omega(\Gamma)}$ takes the same role as that of $G_N(q,\omega)$ for the original lattice. As we can split further each of these new chains into Ω and Γ sub-sublattices, it is again possible to express both $G_N^{(\Omega)}(q,\omega)$ and $G_N^{(\Gamma)}(q,\omega)$ in the form of Eq. (7). Thus we have

$$G_N(q,\omega) = p_{(\Omega\Omega)} G_N^{(\Omega\Omega)}(q,\omega) + p_{(\Omega\Gamma)} G_N^{(\Omega\Gamma)}(q,\omega) + p_{(\Gamma\Omega)} G_N^{(\Gamma\Omega)}(q,\omega) + p_{(\Gamma\Gamma)} G_N^{(\Gamma\Gamma)}(q,\omega). \tag{8}$$

Here we denote the two branches resulting from Ω sublattice as $(\Omega\Omega, \Omega\Gamma)$, while those from Γ-sublattice as $(\Gamma\Omega, \Gamma\Gamma)$. The coefficients can be written as $p_{(\mu\nu)} = p_{(\mu)} p_{(\nu)}$, with $\mu, \nu = \Omega$ or Γ.

If we continue the splitting procedure it will give rise to a tree like structure and it is possible to label each sublattice by its path in this tree. In other words, we label a sublattice by specifying the sequence of Ω and Γ branches that constitute the path leading to the sublattice. The idea of above labeling comes from the fact that this branching process actually gives a family classification [12] for the sites of the PD chain, and we can consider this tree as the genealogical tree for this lattice. So finally we can write $G_N(q,\omega)$ as

$$G_N(q,\omega) = \sum_{all\ \ paths} p_{(path)} G_N^{(path)}(q,\omega), \tag{9}$$

where the sum is over all possible paths in the genealogical tree for a given number of branching. We terminate each path in the genealogical tree using the criteria that the corresponding renormalized coupling constants k_L and k_S flow to zero at this stage of iteration. In this limit the computation of each term in the Eq. (9) becomes trivial (see Eq. (3)) and one can express every $G_N^{(path)}$ into the following general form

$$G_N^{(path)} = -\left(x_\alpha F^*_\alpha/\epsilon^*_\alpha + x_\beta F^*_\beta/\epsilon^*_\beta + x_\gamma F^*_\gamma/\epsilon^*_\gamma\right)\ , \tag{10}$$

where ϵ_i^*'s and F_i^*'s represent the appropriate renormalized parameters, and x_α, x_β and x_γ are the concentrations of α, β and γ sites in the PD chain. From $G_N(q,\omega)$ the dynamic structure factor can be obtained from Eq. (1).

The merit of this scheme is that one has to generate all possible paths in the genealogical tree using a simple algorithm, then iterate the recursion relations T_Ω or T_Γ sequentially along these paths, and finally determine $S(q,\omega)$ using equations (1), (9) and (10). There is no approximation involved in this method and the dynamic structure factor for quasiperiodic lattices can be obtained with arbitrary accuracy, the accuracy level being set by the smallness of the renormalized values of k_L and k_S .

The dispersion relations for the system can be easily obtained from $S(q,\omega)$ using the fact that the ω and q values corresponding to every non-zero values of $S(q,\omega)$ constitutes a point in the dispersion curve. Thus scanning the entire $\omega - q$ plane for non-zero $S(q,\omega)$ one can get the dispersion curve for the PD chain, and this gives the whole spectrum of normal mode frequencies for the system.

IV. LATTICE MODES AND THE TRANSFER MATRIX METHOD

In this section we describe briefly the transfer matrix method for determining the normal mode vibrational states in a one-dimensional lattice. The equations of motion for classical vibration of the chain are

$$m_i\omega^2 u_i = k_{i,i+1}(u_i - u_{i+1}) + k_{i,i-1}(u_i - u_{i-1}), \tag{11}$$

where u_i is the displacement of the ith atom. In the transfer matrix method one can cast the above equation in the following matrix form,

$$\begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} = \begin{pmatrix} \epsilon_i/k_{i,i+1} & -k_{i,i-1}/k_{i,i+1} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_i \\ u_{i-1} \end{pmatrix} \equiv M_i \begin{pmatrix} u_i \\ u_{i-1} \end{pmatrix}. \tag{12}$$

In any normal mode, the displacement u_n of any arbitrary atom n can be obtained from the product of a series of transfer matrices $M_{n-1}M_{n-2}\cdots M_2M_1$ by specifying the initial displacements u_1 and u_0. However, in this technique the determination of the amplitudes at various sites requires a prior knowledge of the normal mode frequency. Since the study of the structure factor gives the entire normal mode frequency spectrum, we can characterize the localized or delocalized nature of the lattice modes in quasiperiodic systems from the asymptotic behavior of the amplitudes at large distances.

At this stage, it is worthwhile to mention that in the PD chain α-type sites always occur in pairs, and an analysis of this dimmer-type correlation provides an understanding about the extended nature of the electronic eigenfunctions in quasiperiodic and disordered systems [5,17]. In a recent work, Dominguez-Adame et al. [14] have shown that this dimmer-type correlation determines the special frequency at which delocalized vibrational mode can exist even in a disordered one-dimensional chain. For a PD chain there are three types of transfer matrices M_α, M_β and M_γ corresponding to the α, β and γ sites in the lattice and it is easy to show that for $\epsilon_\alpha = 0$, apart from a constant phase factor, the total transfer matrix across the PD chain simply reduces to that of a perfectly periodic chain with alternating β and γ atoms. Consequently the system supports delocalized vibrational mode for the frequency ω which satisfies the equation $\epsilon_\alpha = 0$. Since this $\alpha-\alpha$ pairing is present in all the subsequent renormalized lattices, in principle one can determine the full frequency spectrum for delocalized modes by solving the equations $\epsilon_\alpha = \epsilon_\alpha^{'} = \epsilon_\alpha^{''} \cdots = 0$. However, as pointed out earlier, the renormalized ϵ_α's are polynomials in ω, and the degree of the polynomial increases very rapidly with the progress of iteration. So it becomes practically impossible to solve these high degree equations with adequate accuracy. Thus dimmer approach turns out to be inefficient for obtaining the frequency spectrum of the delocalized modes. On the other hand, the dynamic structure factor gives the entire spectrum of normal mode frequencies without much effort and we can easily determine the nature of the normal modes using transfer matrix method.

V. RESULTS AND DISCUSSIONS

With the above background we shall now present in this section the results for some specific cases of the PD chain. We begin by considering the on-site model of the PD chain. In the on-site model two types of masses m_A and m_B, connected by identical spring constants, are distributed on a lattice following PD ordering, and the spacing between the atoms are equal. We can recover the on-site model by setting $m_\alpha = m_\gamma = m_A$, $m_\beta = m_B$, $k_L = k_S = k$ and $a_L = a_S = a$. For numerical calculations, we choose $m_A = 2, m_B = 1, k = 1$ and $a = 1$. In the first column of Fig. 2, we have plotted the dynamic structure factor $S(q,\omega)$ as a function of q for three normal mode frequencies, while the amplitudes of the atoms in these normal modes are shown in the second column of the figure. The first, second and third rows of Fig. 2 respectively correspond to the frequencies $\omega_1^2 = 1, \omega_2^2 = 0.38196$ and $\omega_3^2 = 1.54739$ and these frequencies respectively satisfy the conditions $\epsilon_\alpha = 0$, $\epsilon_\alpha^{'} = 0$ and $\epsilon_\alpha^{''} = 0$. Though these normal mode frequencies can be obtained directly from the dynamic structure factor itself, here we have determined them from the above conditions for getting better numerical accuracy. This figure clearly depicts that for the on-site model, the dynamic structure factor $S(q,\omega)$ becomes a periodic function in wavevector q. From Fig. 2a, 2c and 2e we see that the peaks in $S(q,\omega)$ corresponding to the frequencies ω_1, ω_2 and ω_3 occur respectively at $q = (2n+1)\pi/2$, $(2n+1)\pi/4$ and $(2n+1)\pi/8$, where $n = 0, 1, 2\cdots$. Also the corresponding normal modes display periodicity of periods 4, 8 and 16 in units of the lattice spacing.

Now we shall discuss quite elaborately the underlying physical reason for this periodicity in the dynamic structure factor of the PD chain. For this purpose we restrict ourselves only to the frequency $\omega = \omega_1$. The frequency ω_1 is a root of the equation $\epsilon_\alpha = 0$, and as mentioned earlier, for this frequency one can effectively map the PD chain into an ordered binary chain composed of alternating β and γ type atoms. The dynamic structure factor and the dispersion relation for this periodic lattice are respectively given by

$$S(q,\omega) = -\mathrm{Im}\left[\frac{\epsilon_\beta + \epsilon_\gamma + 2(k_L + k_S)\cos qa}{2(\epsilon_\beta\epsilon_\gamma - k_L^2 - k_S^2 - 2k_Lk_S\cos 2qa)}\right] \tag{13}$$

and

$$\begin{aligned}\omega^2 = (1/2m_\beta m_\gamma)\{&(k_L + k_S)(m_\beta + m_\gamma) \pm [(k_L + k_S)^2(m_\beta - m_\gamma)^2 \\ &+ 4m_\beta m_\gamma(k_L^2 + k_S^2 + 2k_Lk_S\cos 2qa)]^{1/2}\}.\end{aligned} \tag{14}$$

Setting $\omega = \omega_1$, $m_\beta = 1$, $m_\gamma = 2$ and $k_L/k_S = 1$ in Eq. (13), in order to afford a comparison with the above results presented in Fig. 2, we see that the positions of the peaks in $S(q,\omega)$ for this periodic binary chain are situated

at $q = (2n+1)\pi/2$. These positions of the peaks are exactly the same as those observed in Fig. 2a for the on-site model of the chain, though their relative intensities may differ. In other words, at $\omega = \omega_1$, the the peaks of $S(q,\omega)$ for the PD chain exactly coincides with that of a periodic lattice whose unit cell contains two atoms β and γ. From this correspondence we can say that the quasiperiodic PD chain supports delocalized vibrational mode for this frequency and the oscillation of atomic displacements in Fig. 2b actually reflects this extended nature of the mode. In a similar fashion the periodicity of $S(q,\omega)$ in Fig. 2c and Fig. 2e can be explained, and we see that for these cases the dynamic structure factor resembles that of two other periodic lattices whose unit cells consist of four and eight atoms respectively. Thus as far as the dynamics are concerned, quasiperiodic PD chain effectively behaves like an assembly of periodic lattices with periods 4, 8, $\cdots$ etc. and it is quite natural that the corresponding normal modes are extended. In fact, we have observed that for the present choice of the parameters of the system, every normal mode of the PD chain exactly becomes identical to that of an appropriate periodic lattice.

The above equivalence between the PD chain and a set of periodic lattices become much more apparent from the dispersion relation for the PD chain. We have determined the dispersion relation of the PD chain by scanning the entire $\omega - q$ plane for non-zero values of $S(q,\omega)$ and it has been displayed in Fig. 3. In this figure we have also plotted the dispersion curve (solid lines) of the periodic lattice consisting of two type of atoms β and γ. In the periodic case with alternating β and γ type atoms, we have one acoustic and one optical branch. Fig. 3 shows that there is an acoustic branch in the PD chain which coincides with the acoustic branch of this particular periodic lattice, and both of these lattices have a common Brillouin Zone boundary at $q = \pi/2$. This indicates that there is an acoustic branch of the PD chain which comes from an effective periodic lattice of unit cell size two in terms of the lattice spacing. However, in the case of the PD chain, we observe that there are an infinite number of acoustic branches each having its own characteristic Brillouin Zone, and Fig. 3 clearly shows that the edges of these Brillouin Zones are situated at $q = \pi/4,\ \pi/8,\ \cdots$ etc. In Fig. 3 we have displayed the dispersion curve in the extended Brillouin Zone scheme and Zone boundaries other than those mentioned above correspond to the repetition of the various basic Brillouin Zones. The overlap of the various acoustic branches implies that these Brillouin Zones have a nested structure. Thus it is quite interesting that the quasiperiodic PD chain plays the role of an infinite number of periodic lattices whose unit cell sizes increase as 2^n, where $n = 1, 2, \cdots \infty$. The optical branches of the PD chain are in fact the superposition of all the optical branches of these periodic lattices and naturally it would be quite complex. From our calculations we really observe that the optical branches have a very complex structure (see Fig. 3) and actually there can be infinite number of the optical branches for the PD lattice. We observe the following additional features in the optical branch of the PD lattice. For PD lattice we find a well-defined structure in the region of the $\omega - q$ plane corresponding to the gap of the periodic $\beta - \gamma$ binary chain, which is characteristic of the quasiperiodic order of the chain. Fig. 3 also shows that such a structure is absent for low values of q. This is due to the fact that in this long wave length limit (wavelength $\lambda >> a_L$ or a_S) the detailed structure of the lattice is not very important, and both the periodic $\beta - \gamma$ chain and the quasiperiodic PD chain exhibit similar behavior.

In Fig. 4 we have displayed $S(q,\omega)$ as a function of q for other models of the PD chain including some additional graphs corresponding to the on-site model. The graphs for the on-site model are shown in Fig. 4a and 4b corresponding to the frequencies $\omega^2 = 2.26829$ and $\omega^2 = 1.65555$ respectively. The graphs for the bond-model are shown in Fig. 4c and 4d which has been realized by setting $m_\alpha = m_\beta = m_\gamma$, $k_L \neq k_S$ and $a_L \neq a_S$. In this case we choose $m_\alpha = m_\beta = m_\gamma = 1$, $k_L = 1$, $k_S = 2$, $a_L = 2$ and $a_S = 1$ and the Fig. 4c and 4d respectively correspond to the frequencies $\omega^2 = 2.0$ and $\omega^2 = 3.09447$. In Fig. 4e and 4f we have also presented the results for the most general case of the PD chain and here the parameters are taken as $m_\alpha = 1$, $m_\beta = 2$, $m_\gamma = 3$ (all in arbitrary units), $k_S/k_L = 2$ and $a_L/a_S = 2$. The graphs in Fig. 4e and 4f are plotted for frequencies $\omega^2 = 2.0$ and $\omega^2 = 2.42427$ respectively. The most striking feature is that in every case we observe that $S(q,\omega)$ is always periodic in wave vector q. So we can say that this periodicity is a characteristic feature of the PD lattice and it is quite independent of the specific choice of the parameters of the system.

We have demonstrated the underlying physical reason for this periodicity in $S(q,\omega)$ only for the on-site model of the PD chain, which owes its origin to the fact that for every normal mode frequency one can exactly map the system to various periodic lattices. Similar kind of analysis is also possible in other cases, the unit cell structure being quite complex in these situations. The most interesting consequence of the periodicity of $S(q,\omega)$ with respect to q is that the system supports delocalized vibrational modes even in absence of the translational invariance.

At this stage we would like to make the following remark. It should be noted that there exists a polynomial invariant I associated with the recursion relations Eq. (5) and (6) for the PD chain which is given by [5]

$$I = ((\epsilon_\alpha - \epsilon_\gamma)(\epsilon_\alpha - \epsilon_\beta) - k_S^2 - k_L^2)/(2k_L k_S) + 1. \tag{15}$$

Depending upon the choice of parameters of the system, I may be independent of ω as well as it may be a function of ω. In the electronic case, one normally equates the invariant to zero for finding the energy eigenvalues of the extended states of quasiperiodic systems, provided those energies are allowed ones. Similarly we can obtain the delocalized

normal mode frequencies from the condition $I = 0$. However, we have to check whether the frequencies obtained from the above condition give allowed eigenmodes or not. For $m_\alpha = 1, m_\beta = 2, m_\gamma = 3, k_S/k_L = 2$ and $a_L/a_S = 2$ it is found that the condition $I = 0$ is satisfied for $\omega^2 = 1.5$. But this is not an allowed frequency of the system (see Ref. [14]), which is also confirmed from the calculation of $S(q, \omega)$ and it turns out that it is always zero for every q in this case. However, depending on the choice of the parameters of the system, the condition $I = 0$ may give a few allowed delocalized normal mode frequencies. This condition actually corresponds to the commutation of the transfer matrices for two successive generations of the chain, and thus leads to delocalized states. It should be noted that the commutation conditions for various successive generation always give the same set of frequencies due to the presence of the invariant in this system (see Ref. [7] for details). Our RG analysis, however, shows that an infinite number of delocalized eigenmodes are possible in the PD chain due to $\alpha - \alpha$ pairing at all length scales.

VI. CONCLUSIONS

In conclusion, we should stress that the renormalization group method is the right tool for taking into account the symmetry of quasiperiodic systems and the present RSRG scheme offers a very efficient method for computing the dynamic structure factor of these systems. The merit of the present scheme is that it provides an exact method for the determination of $S(q, \omega)$ of infinite self-similar quasiperiodic lattices, and in practice, one can calculate $S(q, \omega)$ with arbitrary accuracy. This method essentially involves the iteration of certain recursion relations, and so it enormously reduces the computational task. We have applied this method to the quasiperiodic PD chain and obtained several new results. Apart from computing the dynamic structure factor, we have also determined the dispersion relation of this lattice. The most interesting result is the observation of periodicity in $S(q, \omega)$ with respect to q for every normal mode frequency, and this periodicity actually gives the signature for the presence of normal mode vibrations which are delocalized over the entire lattice. A direct consequence of the periodicity of $S(q, \omega)$ is that one can infer about the existence of the delocalized vibrational modes in the system simply by looking for the periodicity in the scattering intensity data from diffraction experiment measurements. Another important outcome of the present work is that the entire spectrum of frequencies for delocalized modes can be obtained very easily from the dynamic structure factor, whereas the determination of the full spectrum by the method of Ref. [14] is practically impossible.

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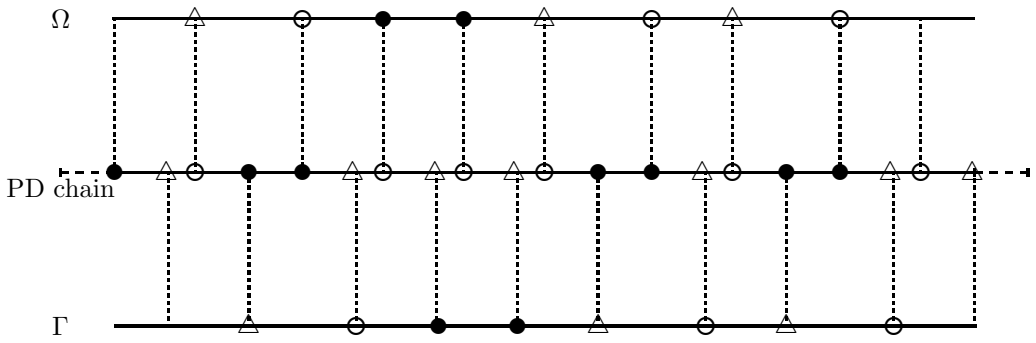
FIG. 1. A section of the period-doubling chain illustrating the sublattice splitting. The symbols •, △ and ◯ respectively represent α, β and γ sites.

FIG. 2. Plot of $S(q,\omega)$ versus q, and u_n versus n for the on-site model with $m_\alpha = m_\gamma = 2, m_\beta = 1$ and $k_L/k_S = 1, a_L/a_S = 1$. First, second and third rows respectively correspond to $\omega^2 = 1.0$, $\omega^2 = 0.38196$ and $\omega^2 = 1.54739$.

FIG. 3. The dispersion relation for the period-doubling lattice with the same parameters as those in Fig. 2.

FIG. 4. Plot of $S(q,\omega)$ versus q. On-site model with parameters $m_\alpha = m_\gamma = 2$, $m_\beta = 1$, $k_L/k_S = 1$ and $a_L/a_S = 1$ for (a) $\omega^2 = 2.26829$ and (b) $\omega^2 = 1.65555$. Bond-model with parameters $m_\alpha = m_\beta = m_\gamma = 1$, $k_S/k_L = 2$ and $a_L/a_S = 2$ for (c) $\omega^2 = 2$ and (d) $\omega^2 = 3.09447$. Mixed model with parameters $m_\alpha = 1$, $m_\beta = 2$, $m_\gamma = 3$, $k_S/k_L = 2$ and $a_L/a_S = 2$ for (e) $\omega^2 = 2$ and (f) $\omega^2 = 2.42427$.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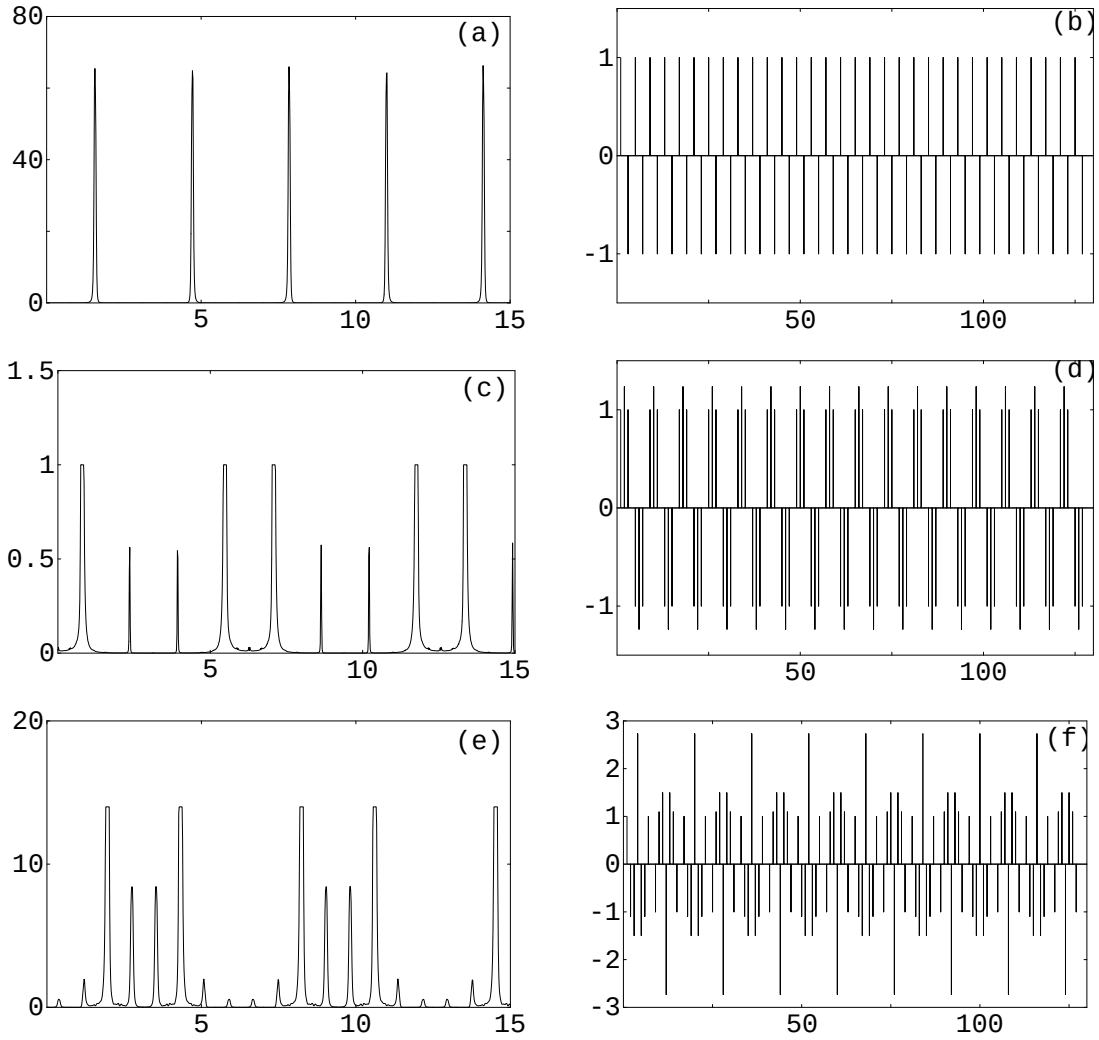
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(d)
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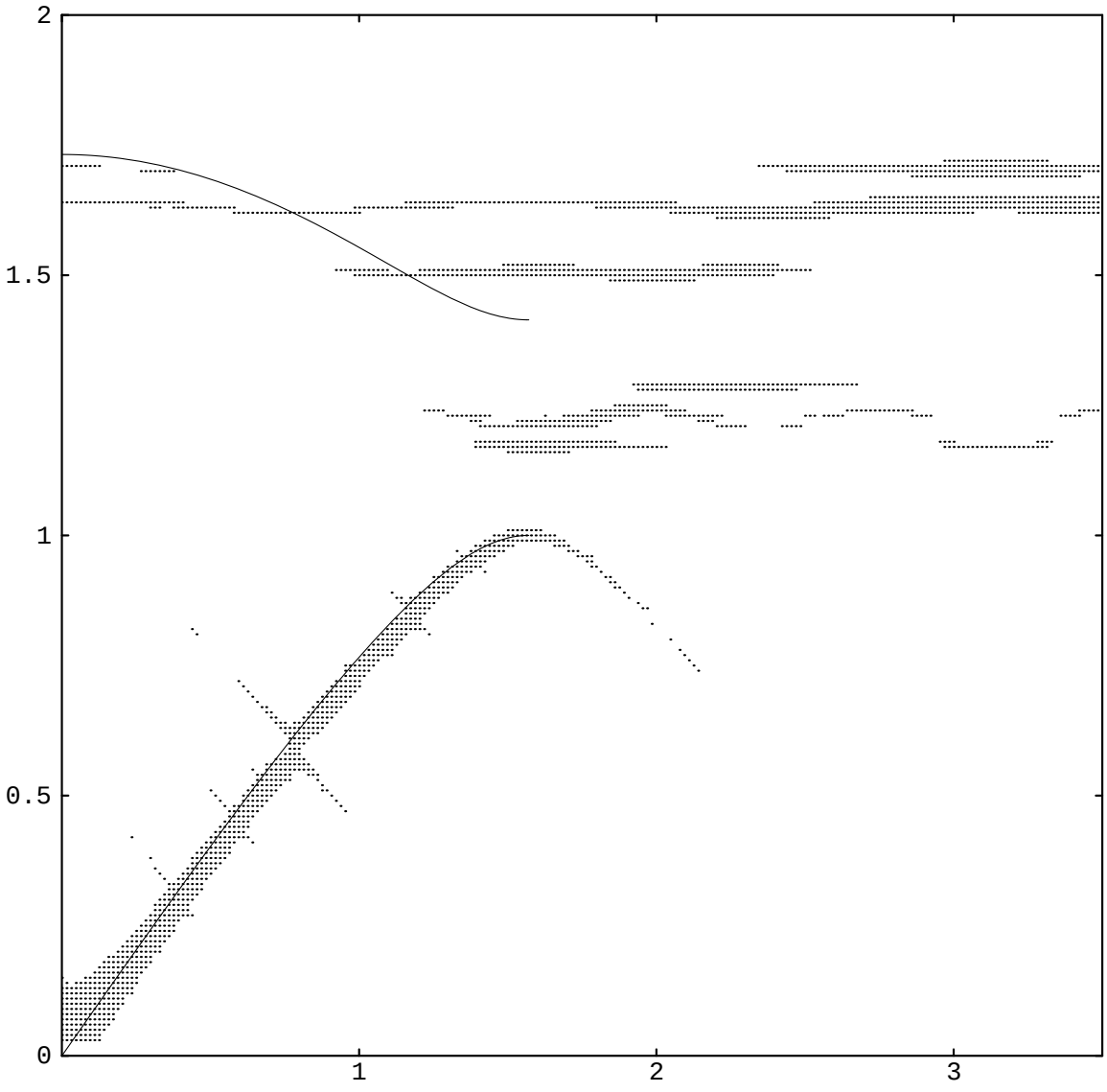
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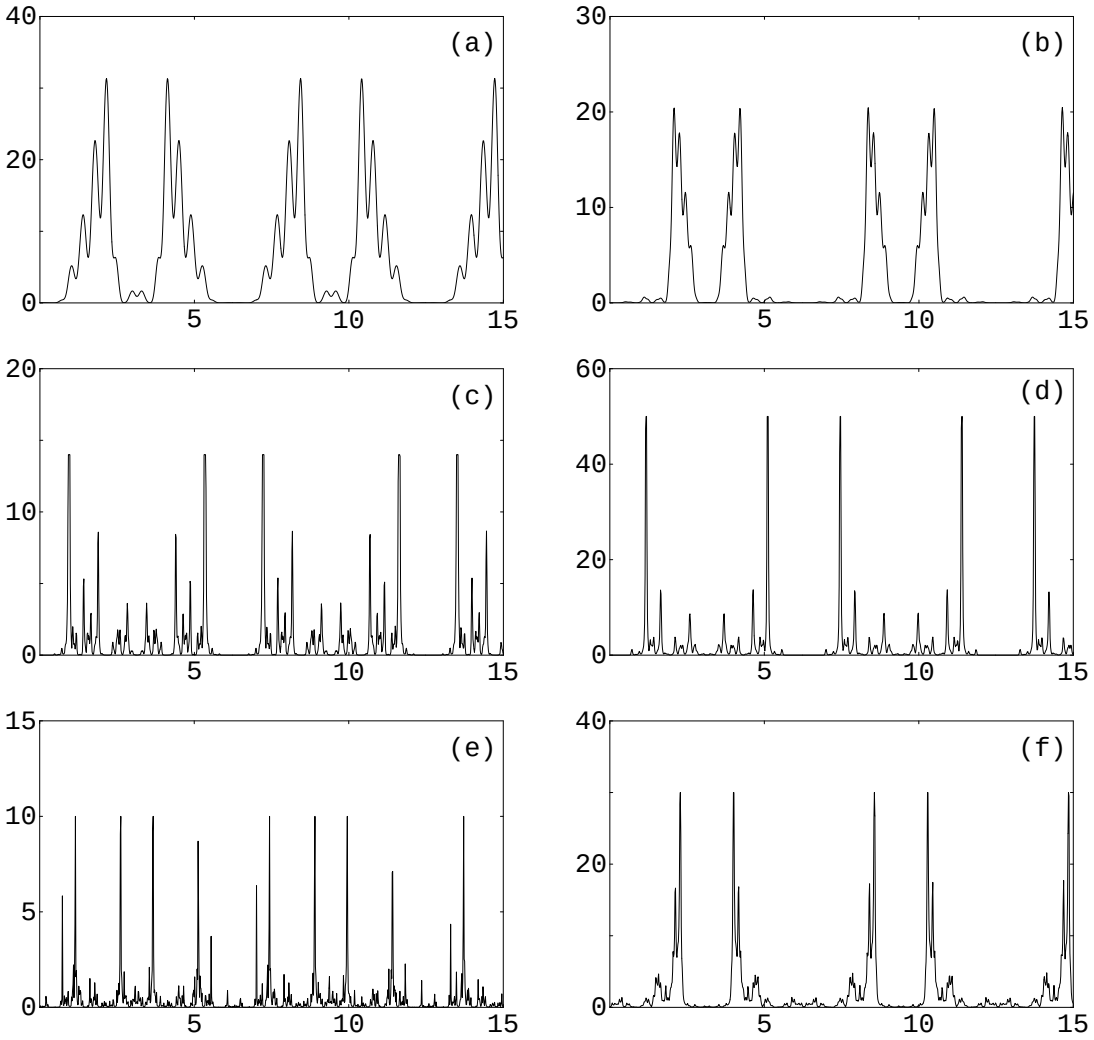
(a)
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